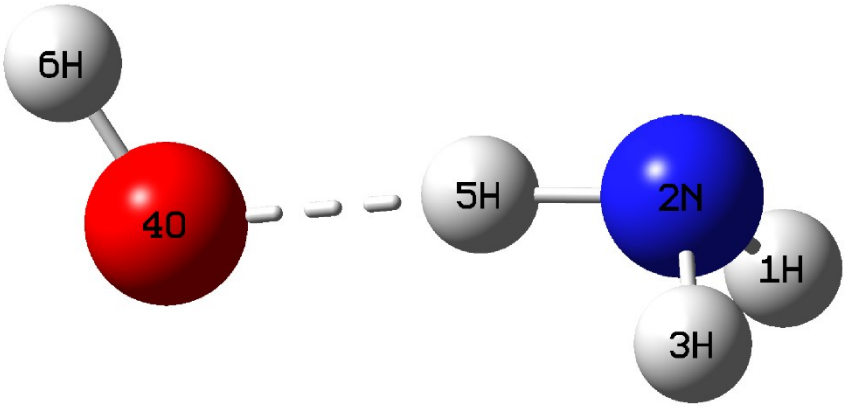
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information

## Quantum calculations of photoelectron spectra of the $OH^-\cdot NH_3$ anion: Implications for $OH + NH_3 \rightarrow H_2O + NH_2$ reaction dynamics

Kohei Saito, Yutaro Sugiura, Takaaki Miyazaki, Yukinobu Takahashi, Toshiyuki Takayanagi*

Department of Chemistry, Saitama University, Shimo-Okubo 255, Sakura-ku, Saitama City, Saitama 338-8570, Japan




$Z_1 = R(N_2–H_1)$
$Z_2 = R(H_3–N_2)$ $Z_6 = \theta(H_3–N_2–H_1)$
$Z_3 = R(O_4–N_2)$ $Z_7 = \theta(O_4–N_2–H_1)$ $Z_{10} = \phi(H_4–N_2–H_1–H_3)$
$Z_4 = R(H_5–N_2)$ $Z_8 = \theta(H_5–N_2–H_1)$ $Z_{11} = \phi(H_5–N_2–H_1–H_3)$
$Z_5 = R(H_6–O_4)$ $Z_9 = \theta(H_6–O_4–N_2)$ $s = \phi(H_6–O_4–N_2–H_1)$

**Figure S1** Definition of internal coordinates used in the anionic potential energy surface construction.

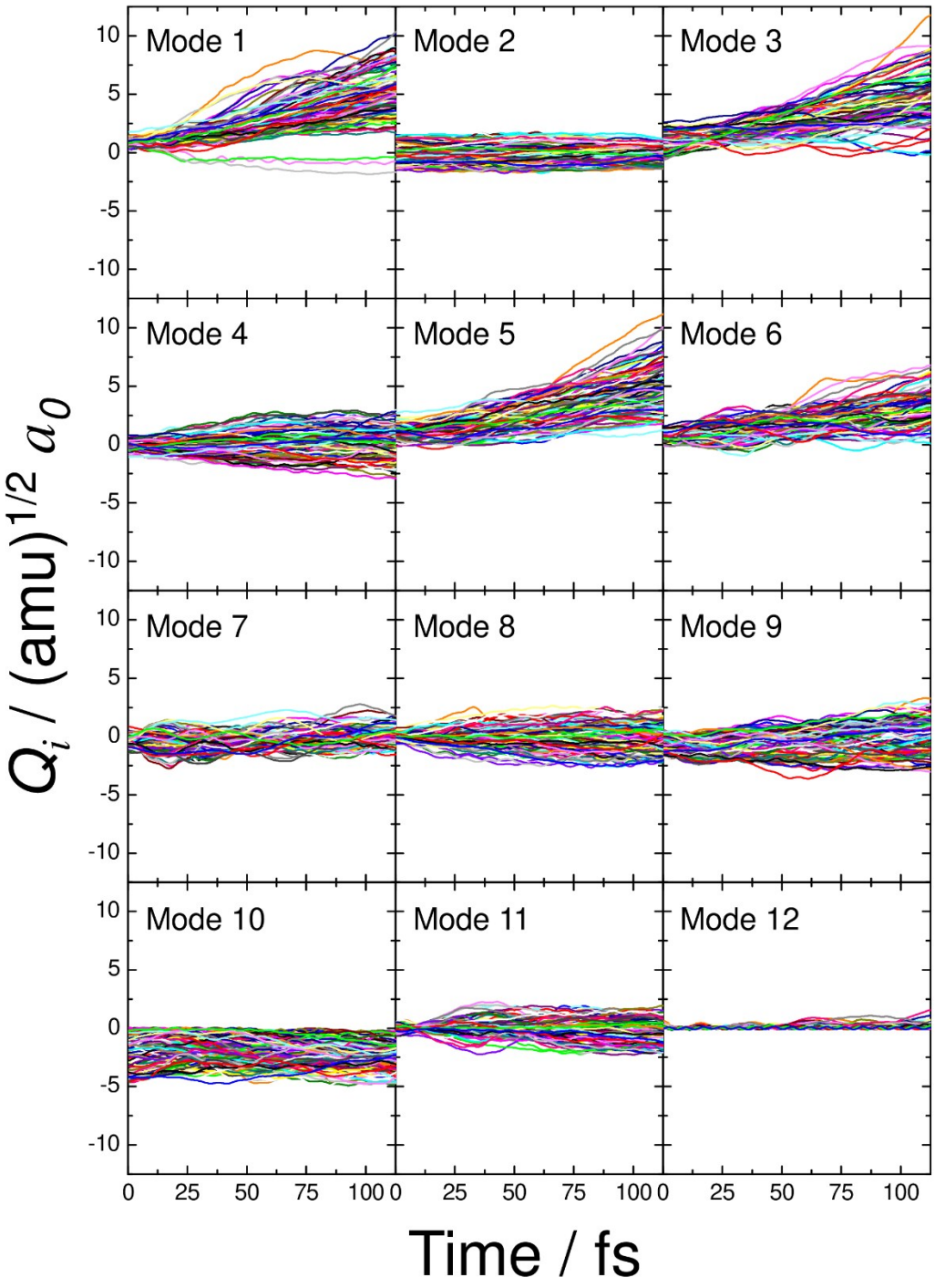



**Figure S2** Time-dependence of the 12 normal mode coordinates along the 100 RPMD trajectories calculated at $T$ = 300 K.

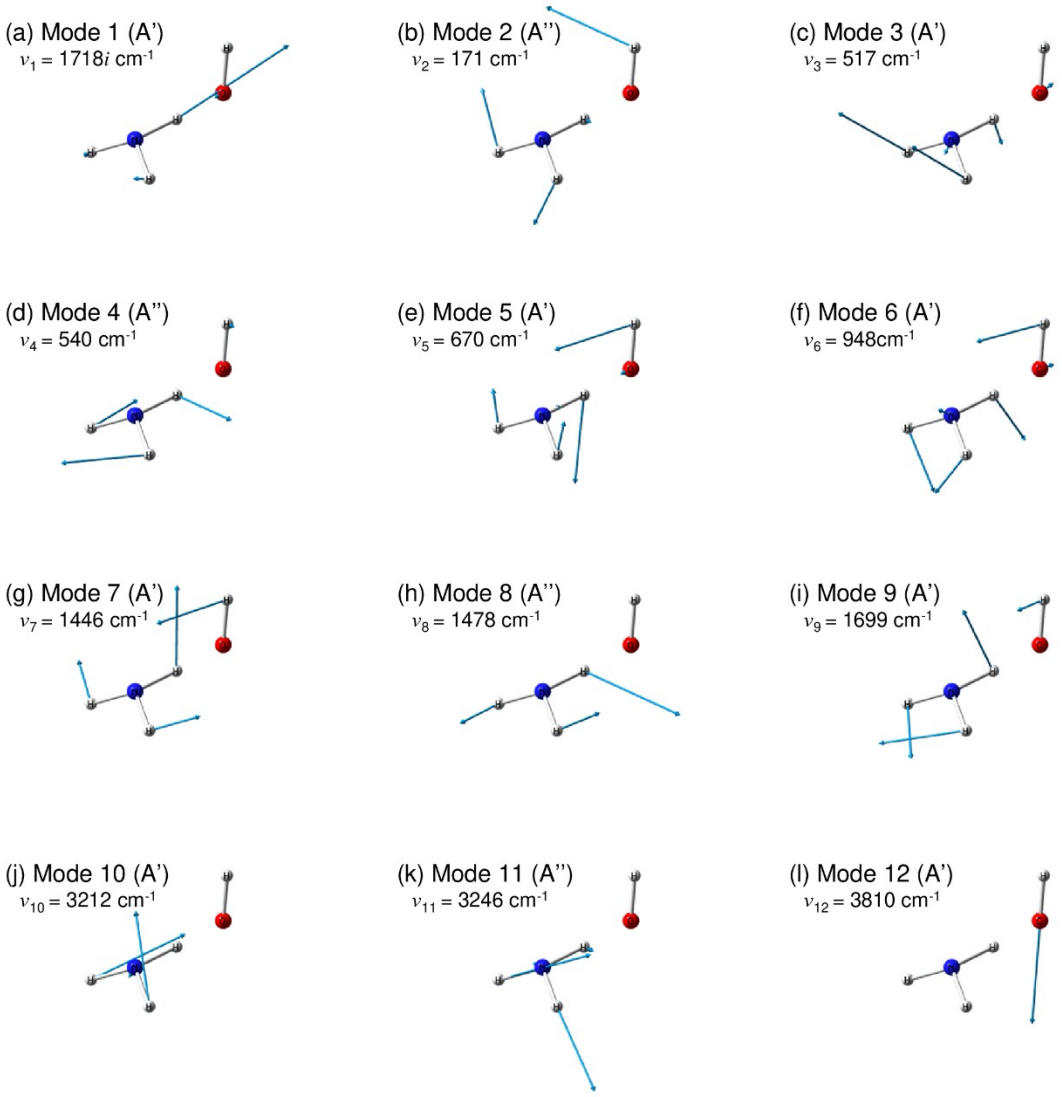



**Figure S3** Normal-mode coordinates obtained from vibrational frequency analysis of the transition-state structure (with anti-configuration) for the $OH + NH_3 \rightarrow H_2O + NH_2$ reaction on the PES-2012 potential energy surface. Mode 1 corresponds to the vibrational mode with an imaginary frequency.

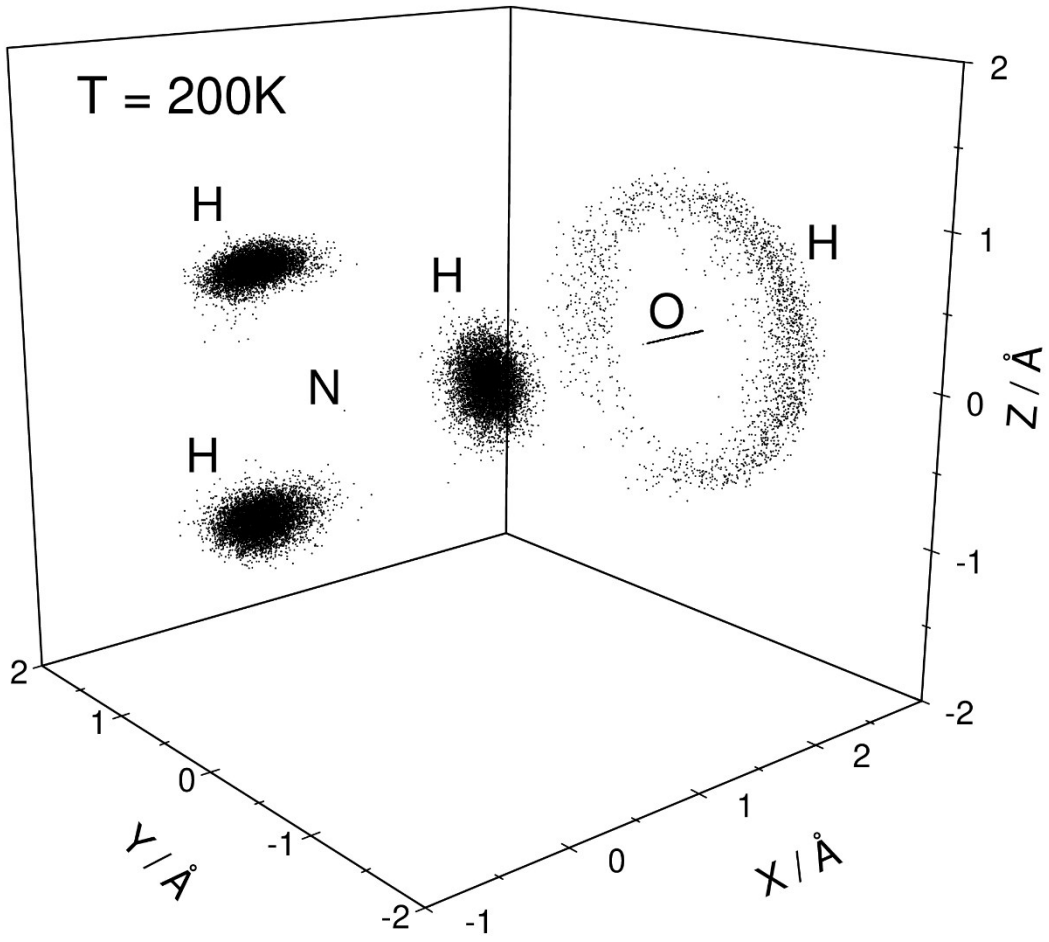



**Figure S4** Three-dimensional perspective plot of the nuclear probability distribution functions of the $OH^{-}\cdot NH_3$ anion calculated from the PIMD simulations at $T$ = 200 K on the interpolated potential energy surface. In this plot, the nitrogen atom is fixed to the coordinate origin and the oxygen atom is always placed on the X-axis. In addition, the midpoint of the two hydrogen atoms (bonding to N) is placed on the X-Y plane.

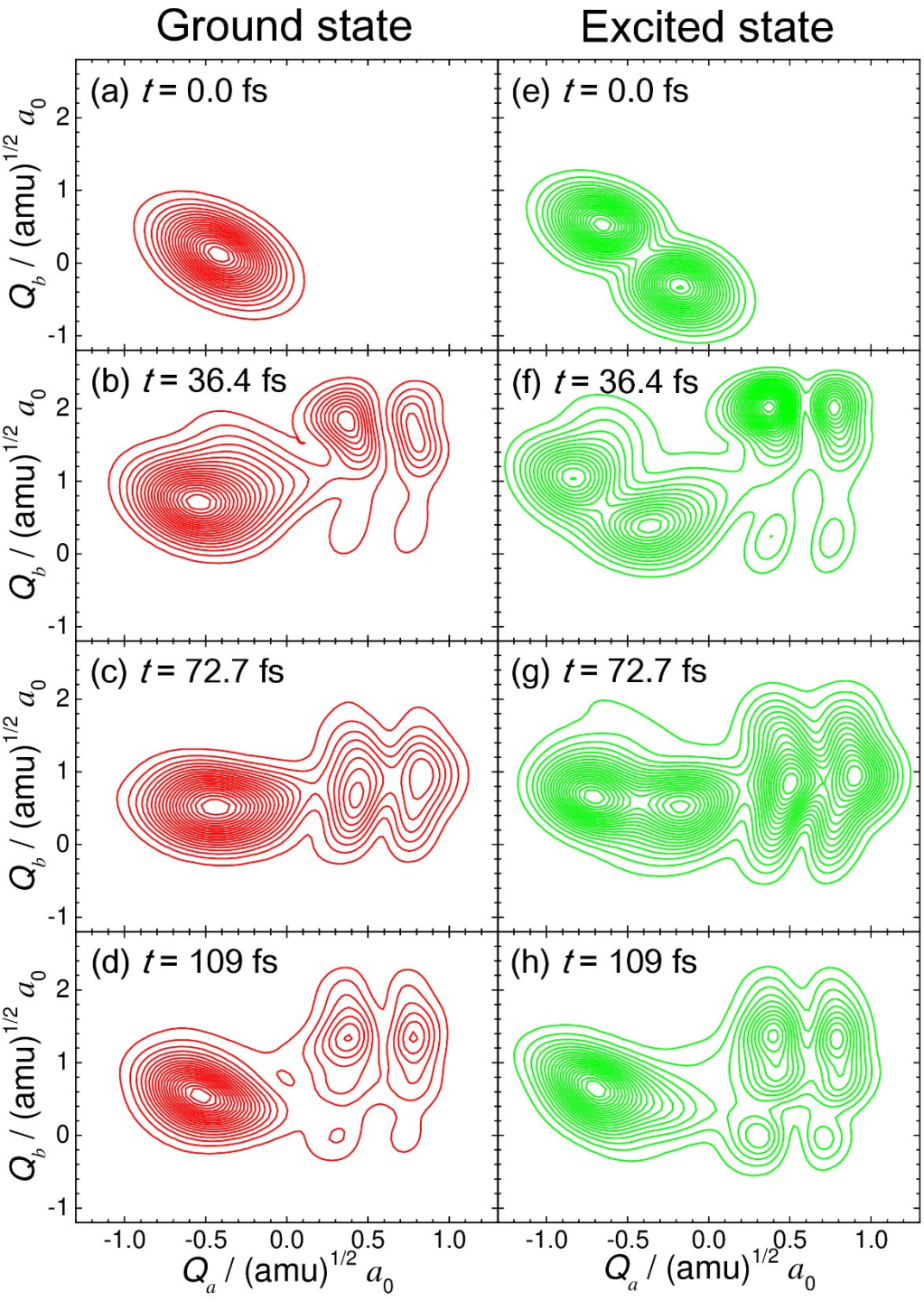



**Figure S5** Time evolution of the wave packet density for the OH + $NH_3$ → $H_2O$ + $NH_2$ reaction system plotted as a function of $Q_a$ and $Q_b$. The wave packet density was integrated over the $Q_c$ and $Q_d$ coordinates. Left and right panels show the wave packet evolutions for the (0000) and (1000) initial anionic states, respectively.

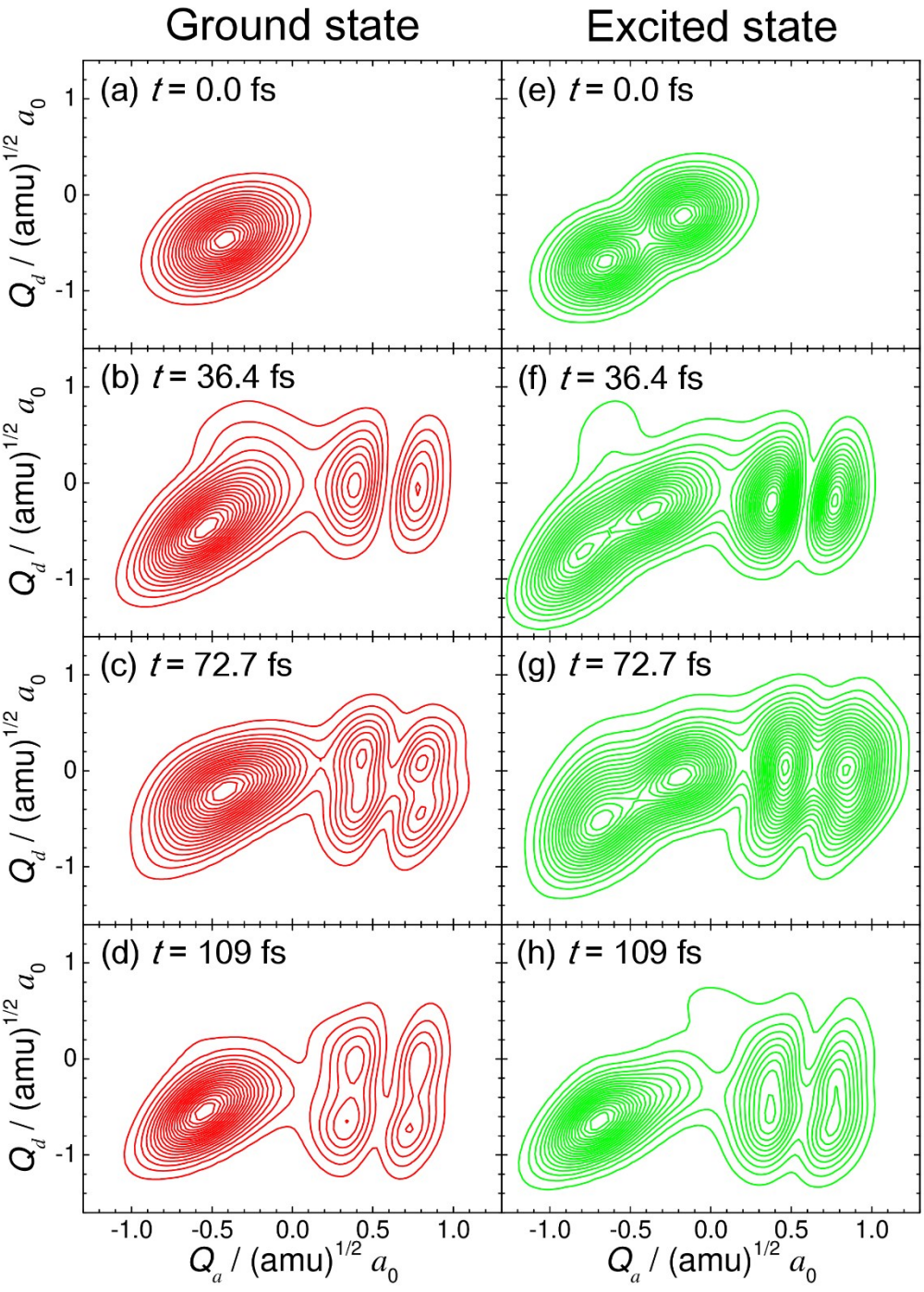



**Figure S6** Time evolution of the wave packet density for the OH + $NH_3$ → $H_2O$ + $NH_2$ reaction system plotted as a function of $Q_a$ and $Q_d$. The wave packet density was integrated over the $Q_b$ and $Q_c$ coordinates. Left and right panels show the wave packet evolutions for the (0000) and (1000) initial anionic states, respectively.